



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:00 PM UTC

PDB ID : 8HUF / pdb_00008huf
Title : B28 in complex with CRM1-Ran-RanBP1
Authors : Sun, Q.; Lei, Y.
Deposited on : 2022-12-23
Resolution : 2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

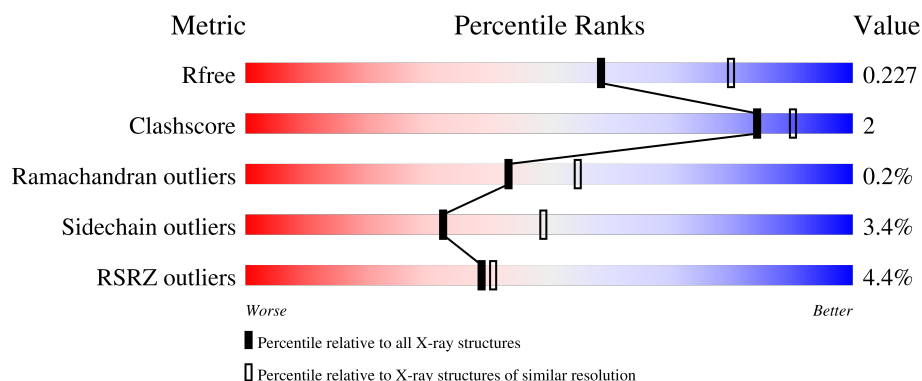
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	216	9% 86% 11%
2	B	140	5% 82% 5% 12%
3	C	1003	3% 91% 8%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 11285 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	1	0
			1680	1084	287	302	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	LEU	GLN	engineered mutation	UNP P62826
A	182	ALA	LEU	engineered mutation	UNP P62826

- Molecule 2 is a protein called YRB1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	123	Total	C	N	O	S	0	0	0
			1007	637	176	189	5			

- Molecule 3 is a protein called CRM1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	997	Total	C	N	O	S	0	1	0
			8061	5181	1327	1511	42			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A6A5PZI8
C	-1	GLY	-	expression tag	UNP A0A6A5PZI8
C	0	SER	-	expression tag	UNP A0A6A5PZI8
C	27	GLU	SER	engineered mutation	UNP A0A6A5PZI8
C	49	GLU	GLN	engineered mutation	UNP A0A6A5PZI8
C	51	VAL	ALA	engineered mutation	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	GLN	deletion	UNP A0A6A5PZI8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	MET	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	GLN	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	GLN	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	ASN	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	TYR	deletion	UNP A0A6A5PZI8
C	?	-	MET	deletion	UNP A0A6A5PZI8
C	?	-	LYS	deletion	UNP A0A6A5PZI8
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	PHE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	ASN	deletion	UNP A0A6A5PZI8
C	?	-	ASP	deletion	UNP A0A6A5PZI8

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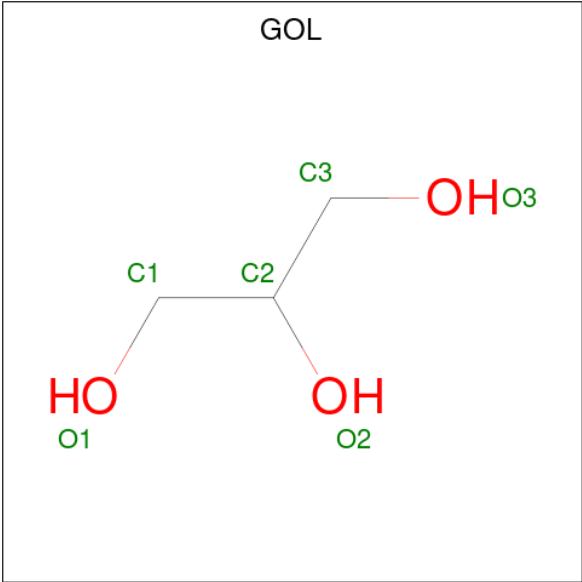
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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	PHE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	LYS	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	ASP	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	537	GLY	ASP	engineered mutation	UNP A0A6A5PZI8
C	539	CYS	THR	engineered mutation	UNP A0A6A5PZI8
C	540	GLU	VAL	engineered mutation	UNP A0A6A5PZI8
C	541	GLN	LYS	engineered mutation	UNP A0A6A5PZI8
C	553	ARG	SER	engineered mutation	UNP A0A6A5PZI8
C	561	GLU	GLN	engineered mutation	UNP A0A6A5PZI8
C	741	THR	ALA	engineered mutation	UNP A0A6A5PZI8
C	1022	CYS	TYR	engineered mutation	UNP A0A6A5PZI8

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

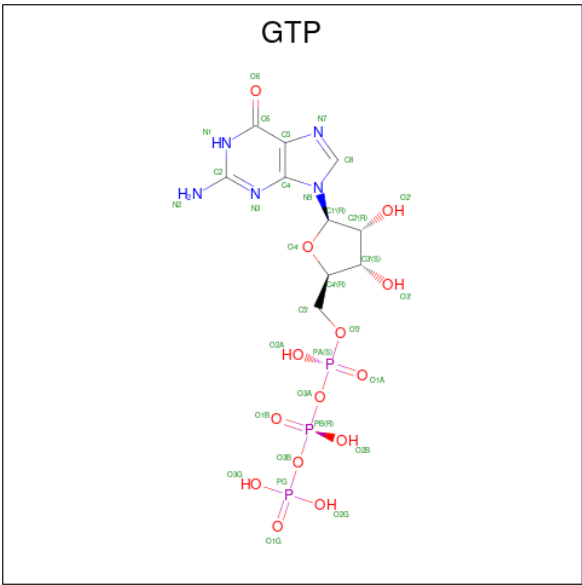
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 7 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Br	0	0
			1	1		

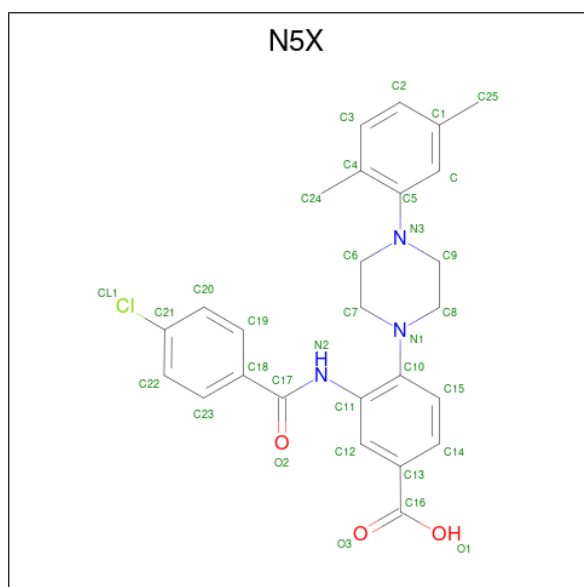
- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Cl	0	0
			1	1		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Na	0	0
			1	1		

- Molecule 10 is 3-[(4-chlorophenyl)carbonylamino]-4-[4-(2,5-dimethylphenyl)piperazin-1-yl] benzoic acid (CCD ID: N5X) (formula: C₂₆H₂₆ClN₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Cl	N	O	0	0
			33	26	1	3	3		

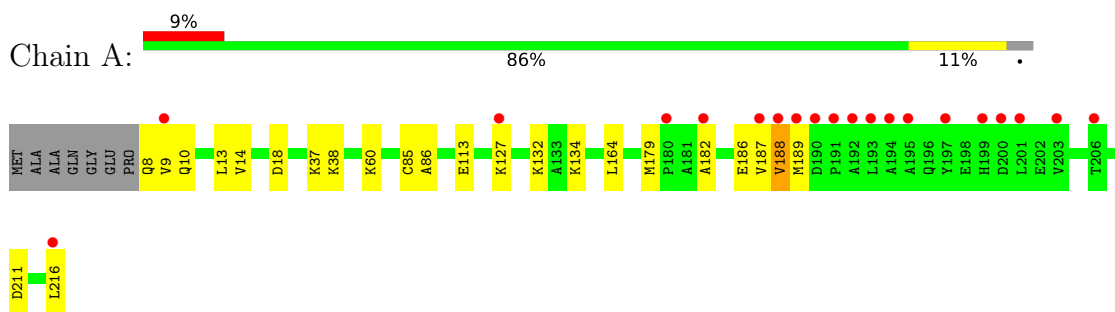
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	97	Total 97	O 97	0	0
11	B	21	Total 21	O 21	0	0
11	C	332	Total 332	O 332	0	0

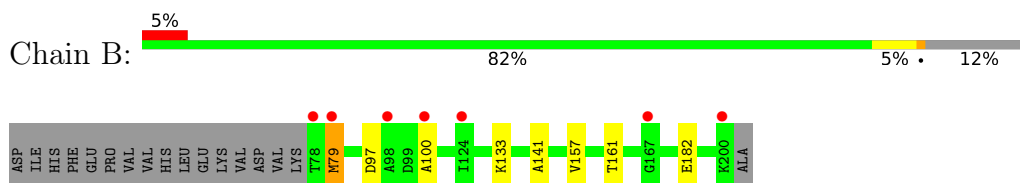
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

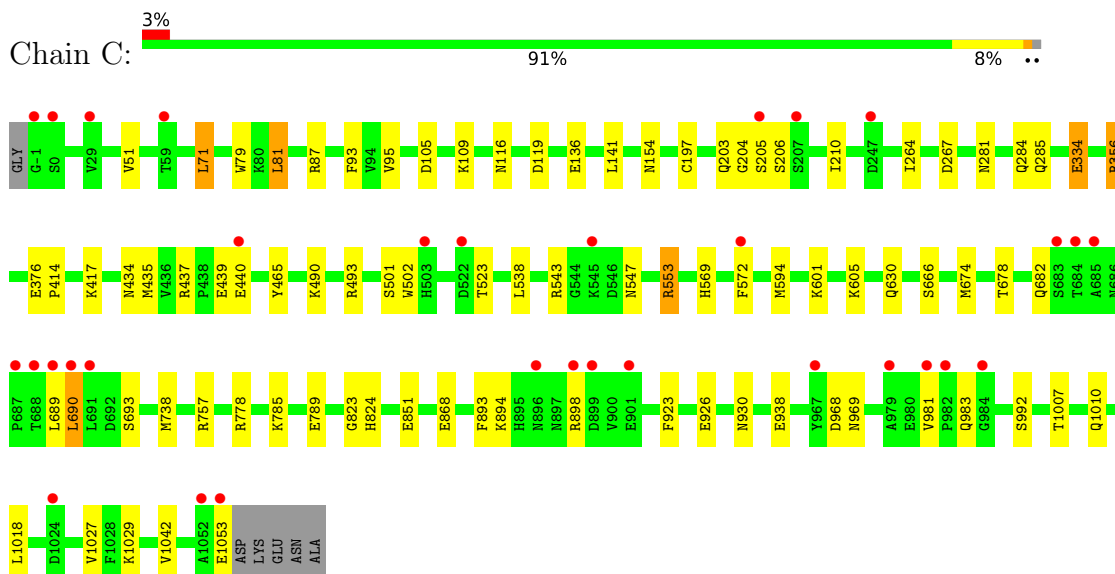
- Molecule 1: GTP-binding nuclear protein Ran



- Molecule 2: YRB1 isoform 1



- Molecule 3: CRM1 isoform 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.36Å 106.36Å 304.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.62 – 2.29 100.42 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.9 (100.62-2.29) 99.9 (100.42-2.29)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.191 , 0.222 0.200 , 0.227	Depositor DCC
R_{free} test set	3999 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11285	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BR, N5X, NA, GTP, GOL, MG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.99	0/1721	1.34	2/2332 (0.1%)
2	B	0.96	0/1024	1.33	0/1367
3	C	0.99	0/8217	1.44	18/11134 (0.2%)
All	All	0.99	0/10962	1.42	20/14833 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	93	PHE	CA-CB-CG	7.43	121.23	113.80
3	C	923	PHE	CA-C-N	5.54	127.65	120.44
3	C	923	PHE	C-N-CA	5.54	127.65	120.44
3	C	523	THR	CA-CB-OG1	-5.42	101.47	109.60
3	C	757	ARG	CA-C-N	5.42	126.00	119.98
3	C	757	ARG	C-N-CA	5.42	126.00	119.98
3	C	893	PHE	CB-CA-C	-5.37	101.55	110.68
3	C	440	GLU	CA-C-N	5.29	127.22	120.56
3	C	440	GLU	C-N-CA	5.29	127.22	120.56
1	A	18	ASP	CA-C-N	5.24	124.95	119.92
1	A	18	ASP	C-N-CA	5.24	124.95	119.92
3	C	823	GLY	CA-C-N	5.19	127.75	120.28
3	C	823	GLY	C-N-CA	5.19	127.75	120.28
3	C	1027	VAL	CA-C-N	5.11	127.08	120.44
3	C	1027	VAL	C-N-CA	5.11	127.08	120.44
3	C	630	GLN	CA-C-N	5.07	127.04	120.44
3	C	630	GLN	C-N-CA	5.07	127.04	120.44
3	C	95	VAL	CA-C-N	5.07	125.57	119.94
3	C	95	VAL	C-N-CA	5.07	125.57	119.94
3	C	868	GLU	CB-CA-C	-5.05	102.31	110.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1680	0	1682	13	0
2	B	1007	0	1008	5	0
3	C	8061	0	8148	36	0
4	A	1	0	0	0	0
5	A	6	0	8	0	0
5	C	12	0	16	3	0
6	A	32	0	12	0	0
7	A	1	0	0	0	0
8	C	1	0	0	0	0
9	C	1	0	0	0	0
10	C	33	0	0	1	0
11	A	97	0	0	1	0
11	B	21	0	0	0	0
11	C	332	0	0	4	0
All	All	11285	0	10874	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197[A]:CYS:SG	11:C:1287:HOH:O	2.37	0.81
3:C:569:HIS:HB3	3:C:572:PHE:HD2	1.53	0.73
3:C:502:TRP:HE1	3:C:547:ASN:HD22	1.38	0.72
3:C:569:HIS:HB3	3:C:572:PHE:CD2	2.30	0.66
3:C:435:MET:HE1	3:C:465:TYR:CE1	2.35	0.62
3:C:204:GLY:HA2	3:C:210:ILE:HD11	1.81	0.61
3:C:682:GLN:HB3	3:C:689:LEU:HD13	1.82	0.61
3:C:1029:LYS:NZ	11:C:1203:HOH:O	2.34	0.60
1:A:189[A]:MET:HG3	2:B:161:THR:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:435:MET:HE1	3:C:465:TYR:CD1	2.40	0.56
3:C:356:ARG:NE	5:C:1103:GOL:O2	2.40	0.54
3:C:334:GLU:H	3:C:334:GLU:CD	2.16	0.53
3:C:502:TRP:HE1	3:C:547:ASN:ND2	2.04	0.53
3:C:894:LYS:NZ	3:C:938:GLU:OE1	2.42	0.53
3:C:824:HIS:ND1	11:C:1204:HOH:O	2.34	0.52
3:C:1007:THR:H	3:C:1010:GLN:HE21	1.57	0.52
1:A:187:VAL:HB	1:A:189[A]:MET:CE	2.39	0.52
1:A:113:GLU:OE1	3:C:116:ASN:ND2	2.44	0.51
3:C:356:ARG:HA	5:C:1103:GOL:H12	1.91	0.51
3:C:553:ARG:HG3	3:C:594:MET:HG2	1.93	0.50
10:C:1105:N5X:N2	10:C:1105:N5X:C8	2.75	0.50
1:A:85:CYS:HB2	1:A:164:LEU:HD22	1.95	0.48
3:C:281:ASN:O	3:C:285:GLN:HG2	2.13	0.48
3:C:690:LEU:HG	3:C:738:MET:HE1	1.95	0.48
3:C:81:LEU:HD13	3:C:1042:VAL:HG11	1.95	0.48
1:A:9:VAL:HA	11:A:484:HOH:O	2.13	0.48
3:C:434:ASN:OD1	5:C:1103:GOL:H31	2.13	0.48
1:A:37:LYS:NZ	1:A:211:ASP:OD1	2.39	0.47
3:C:51:VAL:HG11	3:C:71:LEU:HG	1.98	0.46
1:A:13:LEU:C	1:A:13:LEU:HD23	2.40	0.46
3:C:968:ASP:O	3:C:969:ASN:HB2	2.16	0.46
1:A:179:MET:HE3	2:B:133:LYS:HG2	1.99	0.45
2:B:97:ASP:O	2:B:100:ALA:O	2.34	0.44
3:C:601:LYS:NZ	11:C:1205:HOH:O	2.37	0.44
3:C:926:GLU:O	3:C:930:ASN:ND2	2.51	0.43
3:C:206:SER:O	3:C:210:ILE:HG12	2.17	0.43
3:C:119:ASP:OD2	3:C:154:ASN:ND2	2.49	0.43
1:A:182:ALA:HA	2:B:79:MET:HE3	2.00	0.43
3:C:79:TRP:NE1	3:C:87:ARG:HD2	2.34	0.42
1:A:10:GLN:HA	1:A:60:LYS:O	2.20	0.41
3:C:141:LEU:C	3:C:141:LEU:HD23	2.46	0.41
3:C:435:MET:HE3	3:C:435:MET:HB3	1.79	0.41
3:C:1018:LEU:HD12	3:C:1018:LEU:HA	1.93	0.41
1:A:14:VAL:O	1:A:86:ALA:HA	2.21	0.41
1:A:188:VAL:O	1:A:189[A]:MET:HB2	2.21	0.41
1:A:187:VAL:HG11	2:B:141:ALA:CB	2.50	0.41
3:C:376:GLU:HA	3:C:414:PRO:HD3	1.90	0.40
3:C:437:ARG:CD	3:C:439:GLU:HB2	2.52	0.40
3:C:71:LEU:HD23	3:C:71:LEU:HA	1.93	0.40
3:C:674:MET:O	3:C:678:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	208/216 (96%)	198 (95%)	9 (4%)	1 (0%)	24	31
2	B	121/140 (86%)	115 (95%)	6 (5%)	0	100	100
3	C	996/1003 (99%)	978 (98%)	17 (2%)	1 (0%)	48	60
All	All	1325/1359 (98%)	1291 (97%)	32 (2%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	205	SER
1	A	188	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/184 (98%)	174 (96%)	7 (4%)	28	43
2	B	105/121 (87%)	102 (97%)	3 (3%)	37	55
3	C	912/915 (100%)	881 (97%)	31 (3%)	32	49
All	All	1198/1220 (98%)	1157 (97%)	41 (3%)	32	49

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	38	LYS
1	A	127	LYS
1	A	132	LYS
1	A	134	LYS
1	A	186	GLU
1	A	216	LEU
2	B	79	MET
2	B	157	VAL
2	B	182	GLU
3	C	71	LEU
3	C	81	LEU
3	C	105	ASP
3	C	109	LYS
3	C	136	GLU
3	C	203	GLN
3	C	264	ILE
3	C	267	ASP
3	C	284	GLN
3	C	334	GLU
3	C	356	ARG
3	C	417	LYS
3	C	490	LYS
3	C	493	ARG
3	C	501	SER
3	C	538	LEU
3	C	543	ARG
3	C	553	ARG
3	C	605	LYS
3	C	666	SER
3	C	690	LEU
3	C	693	SER
3	C	778	ARG
3	C	785	LYS
3	C	789	GLU
3	C	851	GLU
3	C	898	ARG
3	C	981	VAL
3	C	983	GLN
3	C	992	SER
3	C	1053	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
3	C	30	GLN
3	C	35	GLN
3	C	111	GLN
3	C	154	ASN
3	C	203	GLN
3	C	274	GLN
3	C	547	ASN
3	C	569	HIS
3	C	928	HIS
3	C	1010	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	N5X	C	1105	-	36,36,36	1.05	1 (2%)	50,51,51	2.17	19 (38%)
6	GTP	A	303	4	33,34,34	0.71	0	50,54,54	0.58	0
5	GOL	C	1103	-	5,5,5	0.12	0	5,5,5	0.44	0
5	GOL	A	302	-	5,5,5	0.09	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	C	1104	-	5,5,5	0.17	0	5,5,5	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	N5X	C	1105	-	-	7/20/30/30	0/4/4/4
6	GTP	A	303	4	-	1/22/38/38	0/3/3/3
5	GOL	C	1103	-	-	4/4/4/4	-
5	GOL	A	302	-	-	1/4/4/4	-
5	GOL	C	1104	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1105	N5X	C21-CL1	3.47	1.82	1.74

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1105	N5X	C4-C5-N3	5.51	123.81	118.83
10	C	1105	N5X	C6-C7-N1	-4.94	100.38	110.78
10	C	1105	N5X	C-C5-N3	-4.45	116.11	122.59
10	C	1105	N5X	C9-N3-C6	3.95	120.46	111.57
10	C	1105	N5X	C22-C21-CL1	3.75	124.89	119.36
10	C	1105	N5X	C8-N1-C7	3.26	118.89	111.57
10	C	1105	N5X	C24-C4-C5	3.09	126.67	122.24
10	C	1105	N5X	C23-C18-C19	2.90	122.25	118.57
10	C	1105	N5X	C8-C9-N3	-2.87	104.75	110.78
10	C	1105	N5X	C14-C13-C12	2.63	122.29	119.25
10	C	1105	N5X	C22-C23-C18	-2.52	118.11	120.80
10	C	1105	N5X	O3-C16-C13	-2.48	114.95	121.46
10	C	1105	N5X	C12-C13-C16	-2.47	115.54	119.96
10	C	1105	N5X	O1-C16-C13	2.45	121.13	114.84
10	C	1105	N5X	C24-C4-C3	-2.39	115.68	120.28
10	C	1105	N5X	C19-C20-C21	2.18	121.43	119.24
10	C	1105	N5X	C7-C6-N3	-2.08	106.42	110.78
10	C	1105	N5X	C18-C17-N2	-2.07	110.87	115.90
10	C	1105	N5X	C20-C21-CL1	-2.04	116.34	119.36

There are no chirality outliers.

All (16) torsion outliers are listed below:

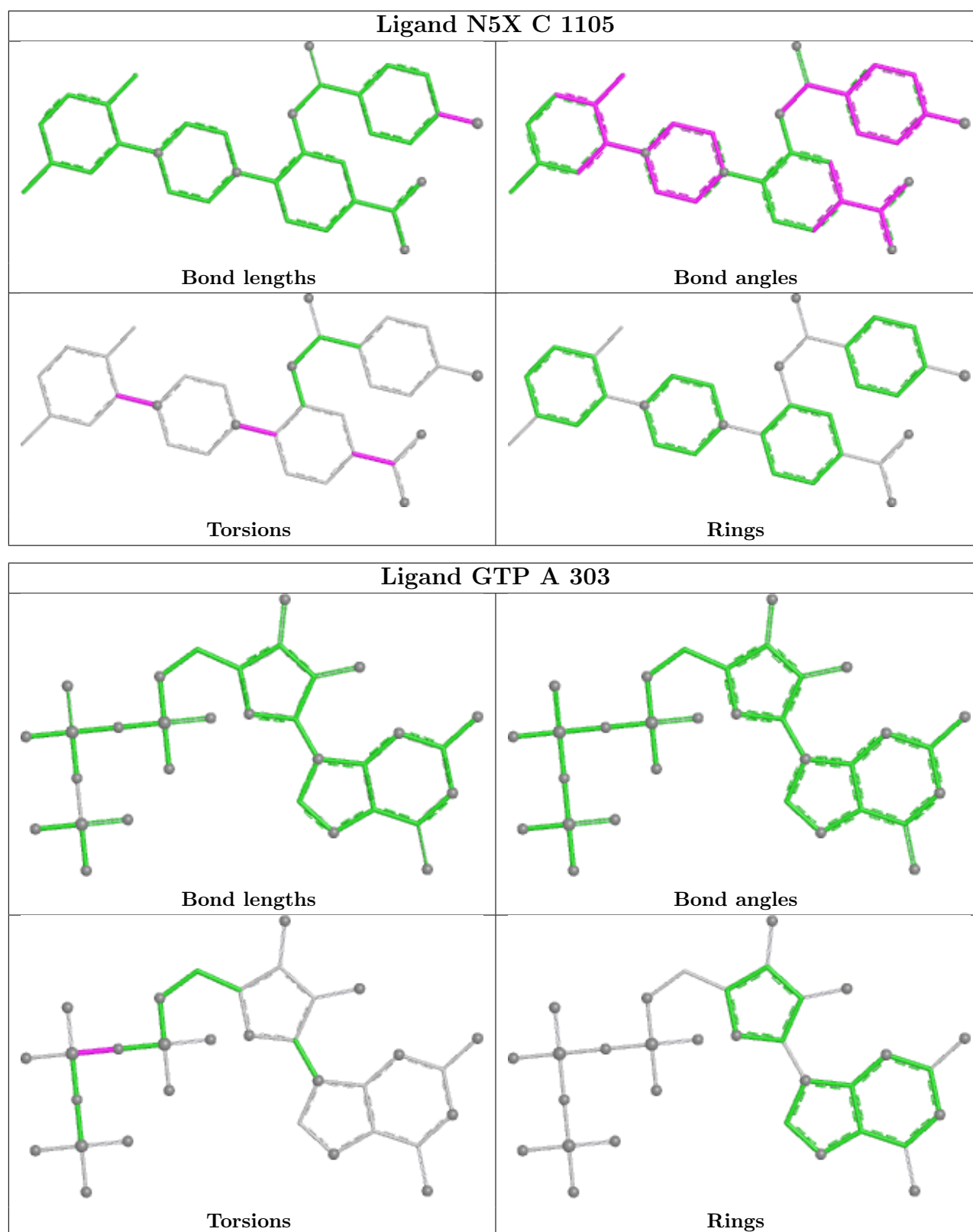
Mol	Chain	Res	Type	Atoms
5	C	1103	GOL	O1-C1-C2-C3
5	C	1104	GOL	O1-C1-C2-C3
10	C	1105	N5X	C12-C13-C16-O1
10	C	1105	N5X	C14-C13-C16-O1
10	C	1105	N5X	C12-C13-C16-O3
10	C	1105	N5X	C14-C13-C16-O3
10	C	1105	N5X	C4-C5-N3-C9
5	C	1103	GOL	O1-C1-C2-O2
5	C	1104	GOL	O1-C1-C2-O2
5	C	1104	GOL	O2-C2-C3-O3
5	C	1103	GOL	C1-C2-C3-O3
10	C	1105	N5X	C11-C10-N1-C8
10	C	1105	N5X	C15-C10-N1-C7
5	C	1103	GOL	O2-C2-C3-O3
5	A	302	GOL	C1-C2-C3-O3
6	A	303	GTP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1105	N5X	1	0
5	C	1103	GOL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/216 (96%)	0.42	20 (9%) 13 15	28, 44, 106, 124	1 (0%)
2	B	123/140 (87%)	0.46	7 (5%) 29 31	43, 57, 86, 109	0
3	C	997/1003 (99%)	0.27	32 (3%) 50 52	25, 47, 77, 114	1 (0%)
All	All	1329/1359 (97%)	0.31	59 (4%) 39 41	25, 48, 80, 124	2 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	PRO	4.7
3	C	689	LEU	4.7
3	C	691	LEU	4.6
1	A	193	LEU	4.1
1	A	188	VAL	3.9
3	C	1053	GLU	3.8
3	C	1052	ALA	3.8
1	A	189[A]	MET	3.5
1	A	187	VAL	3.5
1	A	195	ALA	3.5
1	A	216	LEU	3.4
1	A	197	TYR	3.4
1	A	192	ALA	3.4
3	C	522	ASP	3.3
3	C	690	LEU	3.3
3	C	979	ALA	3.3
2	B	100	ALA	3.1
1	A	9	VAL	3.1
3	C	0	SER	3.0
3	C	684	THR	3.0
3	C	572	PHE	2.9
3	C	687	PRO	3.0
3	C	898	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	78	THR	2.9
3	C	205	SER	2.8
2	B	79	MET	2.7
1	A	200	ASP	2.7
2	B	167	GLY	2.7
1	A	199	HIS	2.6
3	C	899	ASP	2.6
1	A	203	VAL	2.6
3	C	896	ASN	2.5
3	C	-1	GLY	2.5
3	C	967	TYR	2.5
3	C	685	ALA	2.5
3	C	59	THR	2.5
1	A	201	LEU	2.5
3	C	981	VAL	2.4
3	C	29	VAL	2.4
3	C	247	ASP	2.3
3	C	688	THR	2.3
3	C	901	GLU	2.2
3	C	683	SER	2.2
3	C	982	PRO	2.2
2	B	98	ALA	2.2
2	B	200	LYS	2.1
3	C	440	GLU	2.1
3	C	545	LYS	2.1
3	C	1024	ASP	2.1
1	A	180	PRO	2.1
2	B	124	ILE	2.1
3	C	503	HIS	2.1
3	C	984	GLY	2.1
3	C	207	SER	2.1
1	A	190	ASP	2.1
1	A	206	THR	2.0
1	A	182	ALA	2.0
1	A	194	ALA	2.0
1	A	127	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

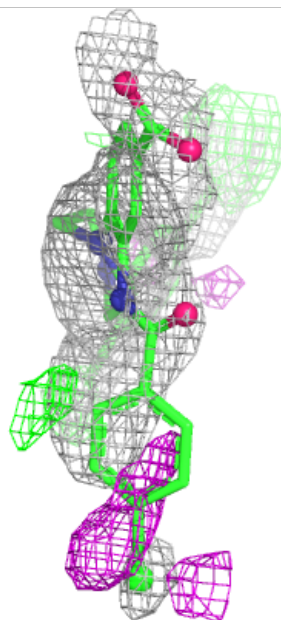
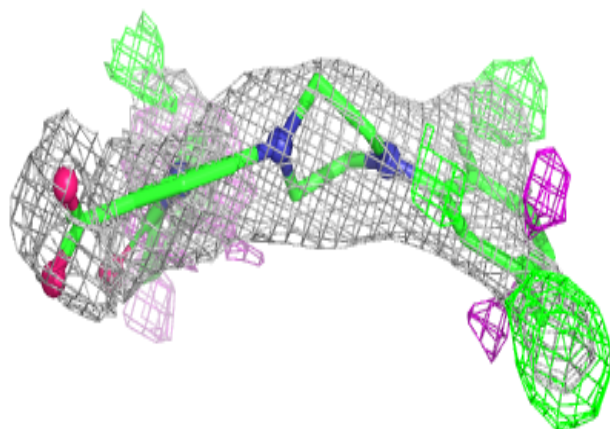
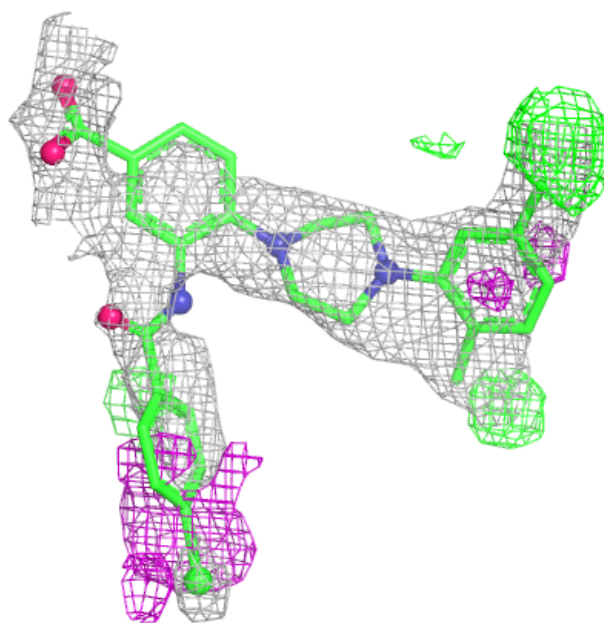
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

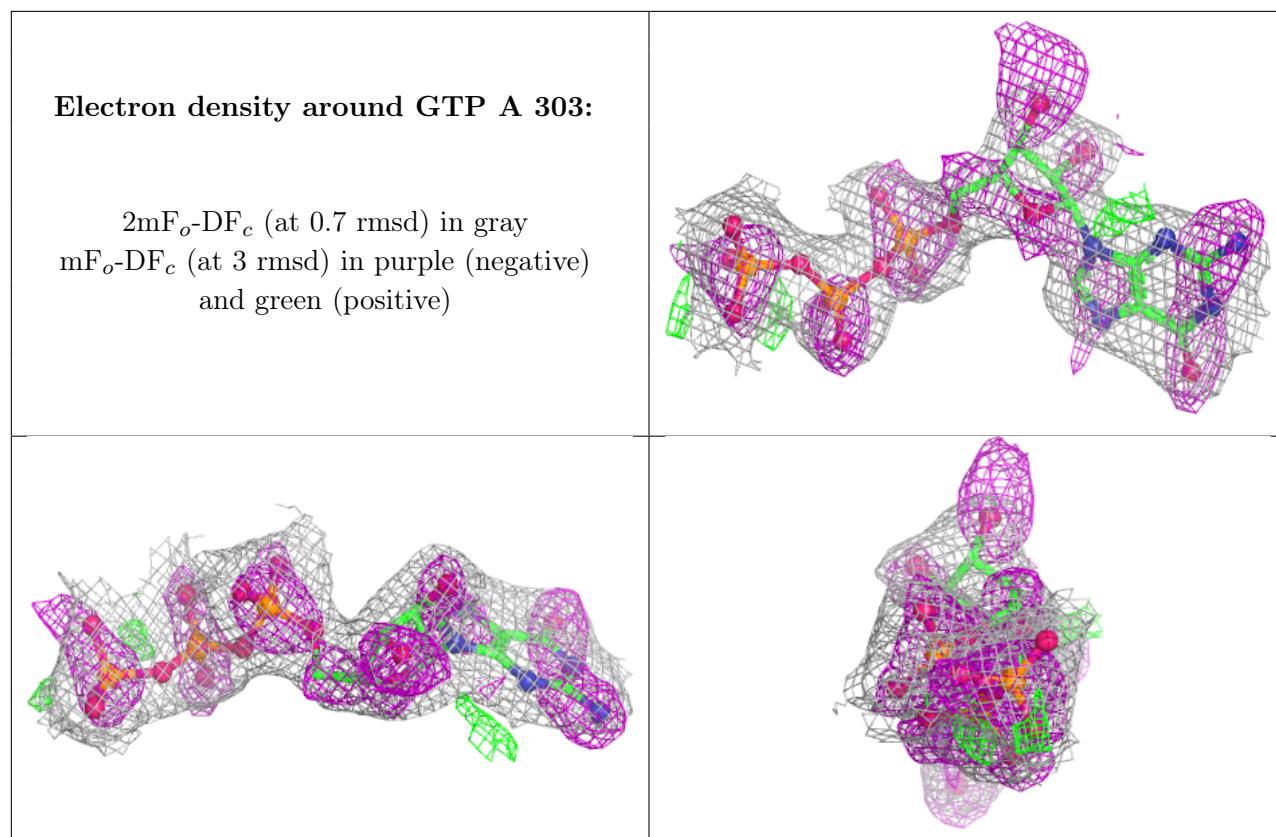
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	N5X	C	1105	33/33	0.70	0.26	80,98,111,111	0
5	GOL	A	302	6/6	0.73	0.23	78,86,89,92	0
5	GOL	C	1104	6/6	0.83	0.14	52,56,58,58	0
5	GOL	C	1103	6/6	0.84	0.16	57,66,68,69	0
9	NA	C	1102	1/1	0.92	0.29	67,67,67,67	0
8	CL	C	1101	1/1	0.95	0.13	68,68,68,68	0
6	GTP	A	303	32/32	0.96	0.08	20,20,20,20	0
7	BR	A	304	1/1	0.97	0.10	82,82,82,82	0
4	MG	A	301	1/1	0.98	0.04	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around N5X C 1105:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.